



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:24 PM UTC

PDB ID : 3AVW / pdb_00003avw
Title : Structure of viral RNA polymerase complex 4
Authors : Takeshita, D.; Tomita, K.
Deposited on : 2011-03-08
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

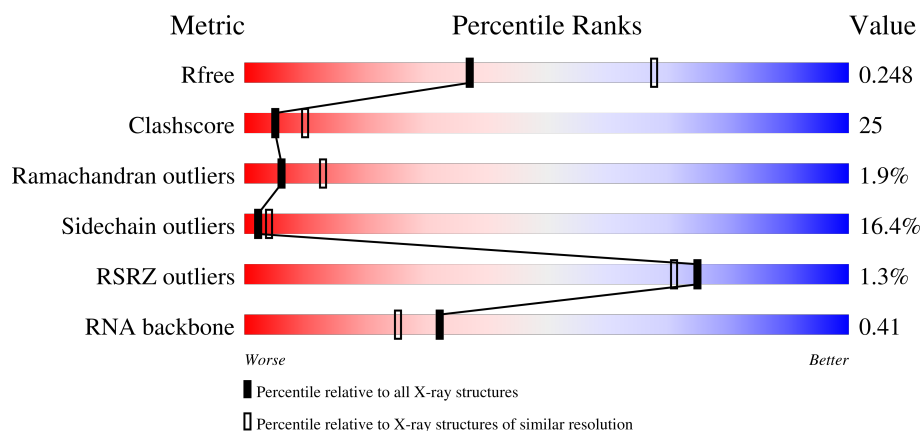
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1289	 51% 33% 9% 7%
2	G	8	 12% 75% 12%
3	T	12	 58% 33% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9843 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1203	Total	C	N	O	S	0	0	0
			9287	5865	1605	1772	45			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	linker	UNP P0A6P3
A	1284	HIS	-	expression tag	UNP Q8LTE0
A	1285	HIS	-	expression tag	UNP Q8LTE0
A	1286	HIS	-	expression tag	UNP Q8LTE0
A	1287	HIS	-	expression tag	UNP Q8LTE0
A	1288	HIS	-	expression tag	UNP Q8LTE0
A	1289	HIS	-	expression tag	UNP Q8LTE0

- Molecule 2 is a RNA chain called RNA (5'-R(*GP*GP*GP*UP*CP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	P	0	0	0
			167	76	31	53	7			

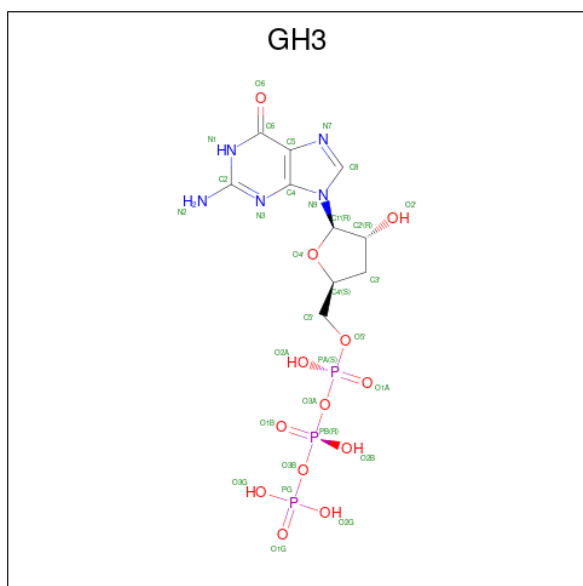
- Molecule 3 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*UP*GP*GP*AP*CP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	12	Total	C	N	O	P	0	0	0
			252	114	46	81	11			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		

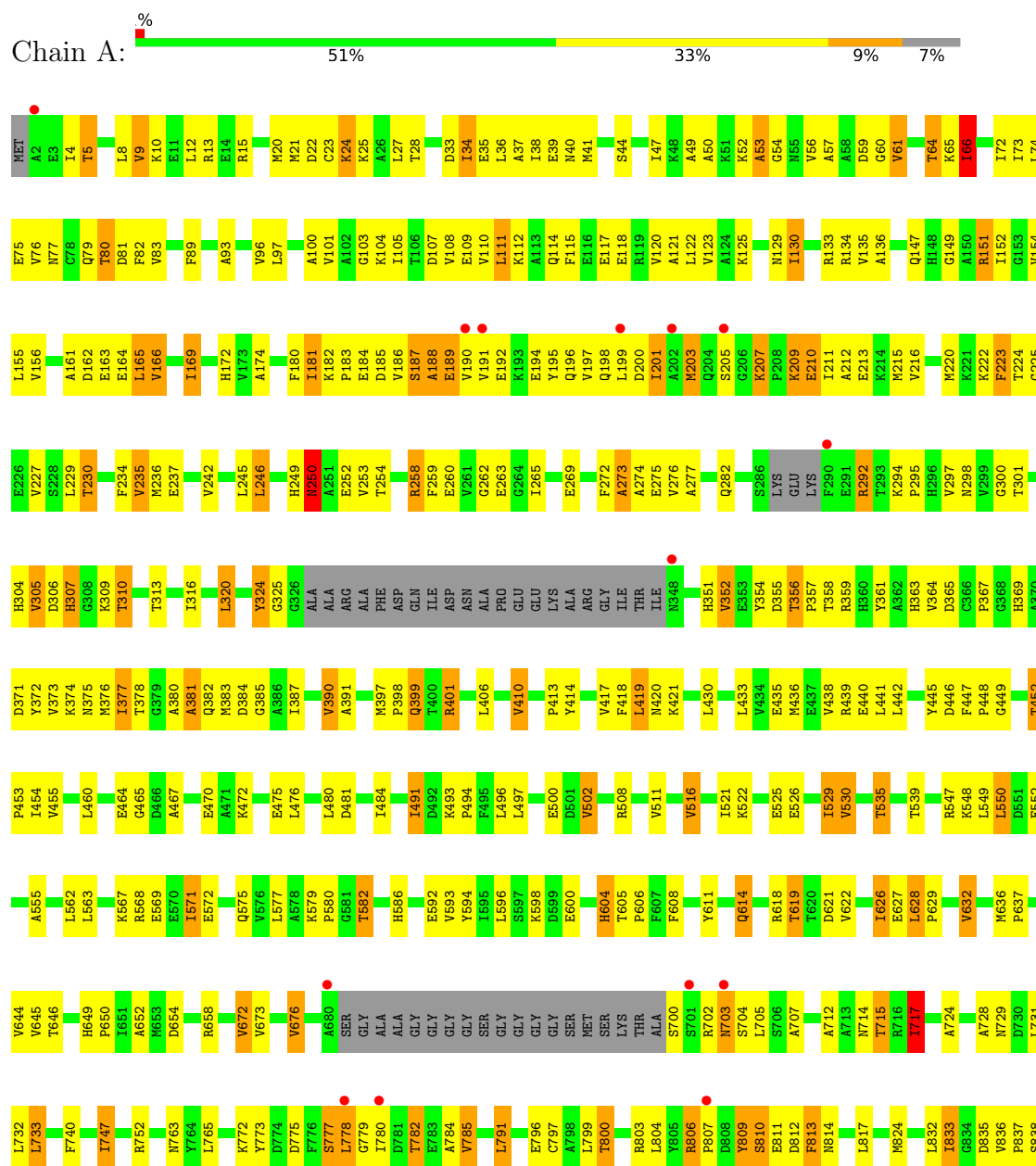
- Molecule 5 is 3'-DEOXY-GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GH3) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

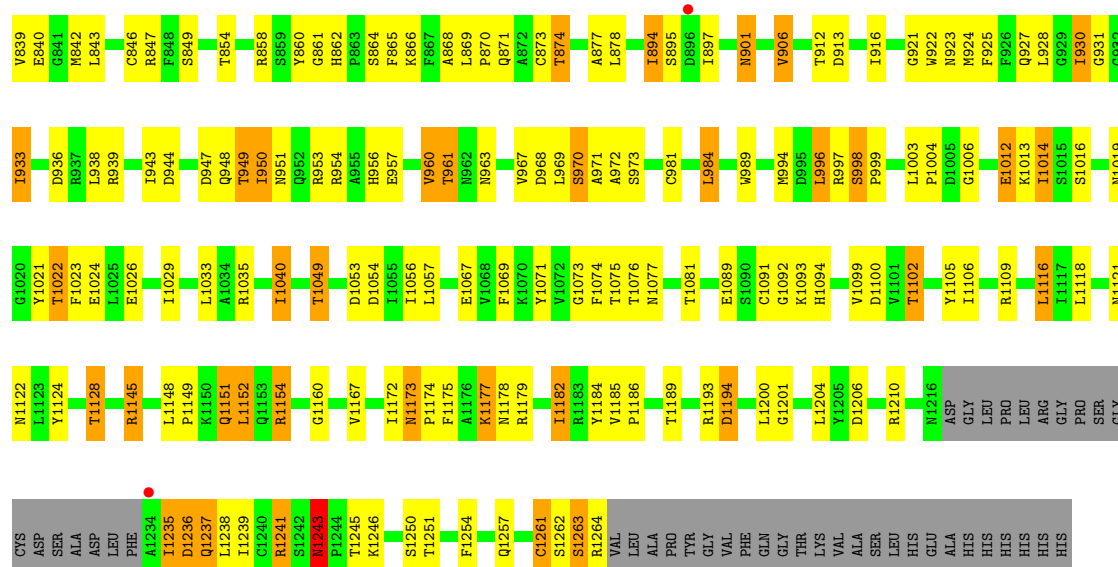


3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase





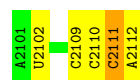
- Molecule 2: RNA (5'-R(*GP*GP*GP*UP*CP*CP*AP*C)-3')

Chain G: 12% 75% 12%



- Molecule 3: RNA (5'-R(*AP*UP*CP*GP*UP*GP*GP*AP*CP*CP*CP*A)-3')

Chain T: 58% 33% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	140.02Å 256.83Å 101.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.60 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (19.99-2.60) 98.5 (19.99-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.201 , 0.253 0.201 , 0.248	Depositor DCC
R_{free} test set	2831 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9843	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GH3, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/9456 (0.0%)	0.94	14/12787 (0.1%)
2	G	0.34	0/186	0.39	0/288
3	T	0.39	0/281	0.43	0/436
All	All	0.60	1/9923 (0.0%)	0.92	14/13511 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	717	ILE	CA-CB	6.42	1.61	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1243	ASN	N-CA-C	8.68	121.67	110.39
1	A	1243	ASN	CA-C-N	6.73	126.75	119.89
1	A	1243	ASN	C-N-CA	6.73	126.75	119.89
1	A	970	SER	N-CA-C	6.17	117.88	111.03
1	A	998	SER	CA-C-N	5.99	125.54	119.19
1	A	998	SER	C-N-CA	5.99	125.54	119.19
1	A	377	ILE	CB-CA-C	-5.80	104.39	111.87
1	A	1006	GLY	N-CA-C	-5.64	107.98	114.69
1	A	207	LYS	CA-C-N	5.29	125.29	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	LYS	C-N-CA	5.29	125.29	119.89
1	A	1235	ILE	N-CA-C	5.27	114.33	106.85
1	A	970	SER	CA-C-N	-5.17	116.07	123.20
1	A	970	SER	C-N-CA	-5.17	116.07	123.20
1	A	66	ILE	N-CA-C	5.12	115.85	107.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	849	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9287	0	9273	471	0
2	G	167	0	87	6	0
3	T	252	0	132	4	0
4	A	2	0	0	0	0
5	T	31	0	12	1	0
6	A	92	0	0	2	0
6	G	3	0	0	0	0
6	T	9	0	0	0	0
All	All	9843	0	9504	478	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (478) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:ASN:HB3	1:A:1022:THR:HG22	1.25	1.15
1:A:491:ILE:HD12	1:A:491:ILE:H	1.17	1.06
1:A:968:ASP:H	1:A:1081:THR:HG22	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:THR:HG23	1:A:953:ARG:HH12	1.27	0.97
1:A:961:THR:HG22	1:A:963:ASN:H	1.26	0.97
1:A:292:ARG:H	1:A:292:ARG:HE	1.04	0.96
1:A:1154:ARG:HG3	1:A:1154:ARG:HH11	1.28	0.95
1:A:806:ARG:O	1:A:806:ARG:HG2	1.69	0.93
1:A:714:ASN:HD21	1:A:1254:PHE:H	1.04	0.92
1:A:399:GLN:H	1:A:399:GLN:HE21	1.18	0.91
1:A:949:THR:HG23	1:A:953:ARG:NH1	1.86	0.90
1:A:862:HIS:HD2	1:A:864:SER:H	1.18	0.90
1:A:1019:ASN:HB3	1:A:1022:THR:CG2	2.02	0.89
1:A:1173:ASN:ND2	1:A:1175:PHE:H	1.72	0.87
1:A:273:ALA:O	1:A:276:VAL:HG12	1.74	0.87
1:A:949:THR:CG2	1:A:953:ARG:HH12	1.87	0.87
1:A:1100:ASP:OD1	1:A:1102:THR:HG23	1.77	0.84
1:A:59:ASP:O	1:A:77:ASN:HB2	1.77	0.84
1:A:448:PRO:O	1:A:452:THR:HG22	1.79	0.83
1:A:1124:TYR:O	1:A:1128:THR:HB	1.79	0.82
1:A:954:ARG:NH1	1:A:1049:THR:HB	1.95	0.82
1:A:49:ALA:HB2	1:A:123:VAL:HG11	1.59	0.82
1:A:491:ILE:H	1:A:491:ILE:CD1	1.93	0.81
1:A:356:THR:HG22	1:A:359:ARG:H	1.45	0.81
1:A:65:LYS:HG2	1:A:101:VAL:HG21	1.62	0.81
1:A:838:SER:HB2	1:A:840:GLU:OE1	1.81	0.80
1:A:611:TYR:HB3	1:A:626:ILE:HD11	1.64	0.79
1:A:378:THR:HG23	1:A:380:ALA:H	1.48	0.79
1:A:324:TYR:CD1	1:A:357:PRO:HD3	2.18	0.78
1:A:301:THR:HB	1:A:363:HIS:NE2	1.98	0.78
1:A:120:VAL:HA	1:A:123:VAL:HG12	1.63	0.77
1:A:21:MET:HA	1:A:21:MET:HE2	1.66	0.77
1:A:375:ASN:HA	1:A:378:THR:HG22	1.65	0.77
1:A:579:LYS:O	1:A:582:THR:HB	1.85	0.77
1:A:20:MET:HE3	1:A:20:MET:HA	1.66	0.77
1:A:491:ILE:HD12	1:A:491:ILE:N	1.98	0.77
1:A:516:VAL:HG22	1:A:555:ALA:HA	1.67	0.77
1:A:372:TYR:CE1	1:A:410:VAL:HG21	2.19	0.76
1:A:307:HIS:CD2	1:A:391:ALA:H	2.04	0.76
1:A:292:ARG:H	1:A:292:ARG:NE	1.83	0.76
1:A:947:ASP:OD1	1:A:949:THR:HB	1.85	0.76
1:A:1173:ASN:C	1:A:1173:ASN:HD22	1.94	0.76
1:A:198:GLN:HA	1:A:201:ILE:HD12	1.67	0.75
1:A:961:THR:CG2	1:A:963:ASN:H	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:HIS:CD2	1:A:864:SER:H	2.05	0.74
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.22	0.74
1:A:714:ASN:ND2	1:A:1254:PHE:H	1.83	0.73
1:A:399:GLN:H	1:A:399:GLN:NE2	1.85	0.73
1:A:250:ASN:N	1:A:250:ASN:HD22	1.87	0.73
1:A:954:ARG:HH11	1:A:1049:THR:HB	1.53	0.72
1:A:212:ALA:O	1:A:216:VAL:HG23	1.89	0.71
1:A:374:LYS:HE3	1:A:594:TYR:CZ	2.26	0.71
1:A:627:GLU:HG2	1:A:644:VAL:HB	1.73	0.70
1:A:25:LYS:O	1:A:28:THR:HG22	1.91	0.70
1:A:1173:ASN:HD22	1:A:1175:PHE:H	1.39	0.70
1:A:420:ASN:ND2	1:A:421:LYS:HG3	2.07	0.70
1:A:249:HIS:C	1:A:250:ASN:HD22	1.99	0.70
1:A:211:ILE:O	1:A:215:MET:HG3	1.92	0.69
1:A:398:PRO:O	1:A:401:ARG:HG2	1.92	0.69
1:A:300:GLY:HA3	1:A:383:MET:SD	2.31	0.69
1:A:399:GLN:HE21	1:A:399:GLN:N	1.89	0.69
1:A:700:SER:O	1:A:1179:ARG:HD3	1.93	0.68
1:A:44:SER:O	1:A:47:ILE:HG22	1.93	0.68
1:A:103:GLY:O	1:A:105:ILE:HG13	1.93	0.68
1:A:796:GLU:O	1:A:800:THR:HG23	1.92	0.68
1:A:80:THR:HG22	1:A:83:VAL:H	1.58	0.68
1:A:187:SER:C	1:A:189:GLU:H	2.02	0.68
1:A:717:ILE:HD13	1:A:717:ILE:C	2.19	0.68
1:A:806:ARG:H	1:A:807:PRO:HD3	1.59	0.67
1:A:372:TYR:HE1	1:A:410:VAL:HG21	1.59	0.67
1:A:310:THR:O	1:A:313:THR:HG22	1.95	0.67
1:A:120:VAL:HA	1:A:123:VAL:CG1	2.24	0.67
1:A:417:VAL:HB	1:A:454:ILE:HG13	1.76	0.67
1:A:1077:ASN:O	1:A:1081:THR:HG23	1.95	0.66
1:A:210:GLU:CD	1:A:210:GLU:H	2.00	0.66
1:A:874:THR:HG22	1:A:877:ALA:H	1.60	0.66
1:A:220:MET:HA	1:A:223:PHE:HB3	1.77	0.66
1:A:442:LEU:HD13	1:A:452:THR:HG21	1.78	0.66
1:A:529:ILE:HD13	1:A:529:ILE:O	1.95	0.66
1:A:1154:ARG:HG3	1:A:1154:ARG:NH1	1.98	0.66
1:A:80:THR:HG23	1:A:82:PHE:H	1.62	0.65
1:A:618:ARG:NH1	1:A:652:ALA:O	2.29	0.65
1:A:901:ASN:C	1:A:901:ASN:HD22	2.04	0.65
1:A:871:GLN:HE21	1:A:921:GLY:HA3	1.61	0.65
1:A:1173:ASN:ND2	1:A:1175:PHE:N	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:HB3	1:A:190:VAL:HG12	1.78	0.65
1:A:811:GLU:HG3	1:A:813:PHE:HB2	1.78	0.65
1:A:8:LEU:HG	1:A:27:LEU:HD21	1.78	0.64
1:A:151:ARG:HH21	1:A:151:ARG:HB2	1.63	0.64
1:A:375:ASN:HA	1:A:378:THR:CG2	2.27	0.64
1:A:526:GLU:HG2	1:A:539:THR:HG22	1.79	0.64
1:A:598:LYS:HD3	1:A:604:HIS:HB2	1.80	0.64
1:A:292:ARG:HE	1:A:292:ARG:N	1.87	0.64
1:A:1182:ILE:HD11	1:A:1184:TYR:CZ	2.33	0.64
1:A:1236:ASP:O	1:A:1239:ILE:HG12	1.98	0.63
1:A:356:THR:HG22	1:A:359:ARG:N	2.13	0.63
1:A:969:LEU:HD21	1:A:1069:PHE:CD2	2.33	0.63
1:A:530:VAL:HG22	1:A:652:ALA:HB2	1.81	0.63
1:A:803:ARG:NH1	1:A:1071:TYR:O	2.32	0.62
1:A:365:ASP:O	1:A:367:PRO:HD3	2.00	0.62
1:A:775:ASP:OD2	1:A:1109:ARG:HD3	1.99	0.62
1:A:309:LYS:HD2	1:A:365:ASP:OD2	1.99	0.62
1:A:181:ILE:HG12	1:A:182:LYS:HG3	1.80	0.61
1:A:75:GLU:O	1:A:75:GLU:HG3	1.99	0.61
1:A:33:ASP:HB3	1:A:36:LEU:HB3	1.81	0.61
1:A:298:ASN:HB2	1:A:382:GLN:HE22	1.65	0.61
1:A:356:THR:HG21	1:A:481:ASP:OD1	2.01	0.61
1:A:870:PRO:HB2	1:A:895:SER:HB3	1.83	0.61
1:A:163:GLU:HG2	1:A:164:GLU:N	2.15	0.61
1:A:529:ILE:HD11	1:A:575:GLN:OE1	1.99	0.61
1:A:500:GLU:CD	1:A:1210:ARG:HH12	2.09	0.60
1:A:183:PRO:HD3	1:A:230:THR:HB	1.84	0.60
1:A:702:ARG:CB	1:A:705:LEU:HB3	2.31	0.60
1:A:930:ILE:HD11	1:A:1021:TYR:CG	2.36	0.60
1:A:24:LYS:HA	1:A:24:LYS:NZ	2.17	0.60
1:A:304:HIS:CD2	1:A:397:MET:HE2	2.37	0.60
1:A:729:ASN:HD21	1:A:740:PHE:H	1.49	0.60
1:A:1077:ASN:C	1:A:1077:ASN:HD22	2.09	0.60
1:A:1094:HIS:H	1:A:1102:THR:HG22	1.67	0.60
1:A:1173:ASN:HD22	1:A:1174:PRO:N	2.00	0.60
1:A:997:ARG:HD2	1:A:1014:ILE:O	2.02	0.59
1:A:1121:ASN:HD21	1:A:1167:VAL:H	1.49	0.59
1:A:649:HIS:HB2	1:A:650:PRO:CD	2.32	0.59
1:A:181:ILE:HG23	1:A:185:ASP:OD1	2.02	0.59
1:A:572:GLU:O	1:A:575:GLN:HG3	2.02	0.59
1:A:195:TYR:HB2	1:A:220:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:O	1:A:320:LEU:HB2	2.03	0.59
1:A:704:SER:HA	1:A:707:ALA:HB3	1.84	0.58
1:A:24:LYS:HA	1:A:24:LYS:HZ2	1.69	0.58
1:A:72:ILE:HG13	1:A:136:ALA:O	2.04	0.58
1:A:96:VAL:HA	1:A:115:PHE:CZ	2.39	0.58
1:A:951:ASN:OD1	1:A:1049:THR:HG23	2.04	0.58
1:A:1245:THR:O	1:A:1246:LYS:HD3	2.03	0.58
1:A:227:VAL:HG22	1:A:227:VAL:O	2.03	0.58
1:A:806:ARG:N	1:A:807:PRO:HD3	2.19	0.58
1:A:356:THR:CG2	1:A:359:ARG:H	2.16	0.57
1:A:894:ILE:HD11	1:A:897:ILE:HB	1.86	0.57
1:A:111:LEU:HA	1:A:114:GLN:HB3	1.85	0.57
1:A:174:ALA:O	1:A:258:ARG:NH1	2.37	0.57
1:A:209:LYS:HE3	1:A:213:GLU:OE2	2.04	0.57
1:A:262:GLY:HA2	1:A:265:ILE:HD12	1.86	0.57
1:A:951:ASN:OD1	1:A:1049:THR:CG2	2.52	0.57
1:A:809:TYR:O	1:A:810:SER:HB2	2.04	0.57
1:A:229:LEU:O	1:A:242:VAL:HB	2.05	0.56
1:A:924:MET:HE1	1:A:928:LEU:CG	2.35	0.56
1:A:968:ASP:N	1:A:1081:THR:HG22	2.10	0.56
1:A:120:VAL:CA	1:A:123:VAL:HG12	2.34	0.56
1:A:529:ILE:HD11	1:A:575:GLN:CD	2.31	0.56
1:A:72:ILE:HD11	1:A:135:VAL:CG2	2.35	0.56
1:A:80:THR:HG23	1:A:82:PHE:N	2.20	0.56
1:A:21:MET:HE1	1:A:430:LEU:HD23	1.86	0.56
1:A:453:PRO:C	1:A:454:ILE:HD12	2.31	0.56
1:A:931:GLY:O	1:A:1024:GLU:HG2	2.06	0.56
1:A:52:LYS:C	1:A:54:GLY:H	2.13	0.56
1:A:385:GLY:HA3	1:A:484:ILE:HD12	1.88	0.56
1:A:1182:ILE:HG12	1:A:1184:TYR:CE2	2.40	0.56
1:A:187:SER:C	1:A:189:GLU:N	2.63	0.55
1:A:276:VAL:HG13	1:A:277:ALA:N	2.21	0.55
1:A:380:ALA:O	1:A:381:ALA:HB2	2.06	0.55
1:A:1177:LYS:HE3	1:A:1177:LYS:HA	1.88	0.55
1:A:1014:ILE:O	1:A:1014:ILE:HD13	2.07	0.55
1:A:73:ILE:HG23	1:A:259:PHE:CE1	2.41	0.55
1:A:800:THR:HG21	1:A:1073:GLY:HA2	1.89	0.55
3:T:2111:C:H5'	3:T:2112:A:OP2	2.07	0.55
1:A:4:ILE:HD11	1:A:28:THR:HA	1.88	0.55
1:A:629:PRO:HD2	1:A:632:VAL:CG1	2.37	0.55
1:A:1160:GLY:O	3:T:2109:C:H4'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:VAL:HG23	1:A:1186:PRO:HD2	1.88	0.55
1:A:34:ILE:HD12	1:A:34:ILE:H	1.72	0.54
1:A:21:MET:HE2	1:A:21:MET:CA	2.36	0.54
1:A:108:VAL:O	1:A:111:LEU:HD23	2.08	0.54
1:A:182:LYS:HB2	1:A:185:ASP:OD2	2.06	0.54
1:A:933:ILE:HG12	1:A:989:TRP:HH2	1.72	0.54
1:A:301:THR:HG22	1:A:365:ASP:HA	1.89	0.54
1:A:439:ARG:NH1	1:A:449:GLY:O	2.40	0.54
1:A:21:MET:HA	1:A:21:MET:CE	2.35	0.54
1:A:1182:ILE:HD11	1:A:1184:TYR:OH	2.06	0.54
1:A:924:MET:HE1	1:A:928:LEU:HG	1.88	0.54
1:A:1206:ASP:O	1:A:1210:ARG:HG3	2.06	0.54
1:A:373:VAL:O	1:A:377:ILE:HG12	2.07	0.54
1:A:13:ARG:C	1:A:15:ARG:H	2.15	0.53
1:A:111:LEU:HD23	1:A:112:LYS:H	1.73	0.53
1:A:249:HIS:C	1:A:250:ASN:ND2	2.66	0.53
1:A:356:THR:HG23	1:A:358:THR:H	1.73	0.53
1:A:163:GLU:HG2	1:A:164:GLU:H	1.70	0.53
1:A:824:MET:HE1	1:A:1040:ILE:CG1	2.38	0.53
1:A:1121:ASN:ND2	1:A:1167:VAL:H	2.06	0.53
1:A:930:ILE:HD11	1:A:1021:TYR:CB	2.39	0.53
1:A:703:ASN:C	1:A:705:LEU:H	2.17	0.53
1:A:981:CYS:SG	1:A:1014:ILE:HG13	2.49	0.53
1:A:351:HIS:CG	1:A:351:HIS:O	2.62	0.53
1:A:874:THR:HG22	1:A:877:ALA:N	2.23	0.53
1:A:182:LYS:HB3	1:A:184:GLU:OE2	2.09	0.53
1:A:161:ALA:HB1	1:A:165:LEU:HB3	1.91	0.52
1:A:199:LEU:O	1:A:203:MET:HG3	2.09	0.52
1:A:1151:GLN:HE21	1:A:1151:GLN:H	1.56	0.52
1:A:833:ILE:HG23	1:A:989:TRP:CE2	2.44	0.52
1:A:861:GLY:O	1:A:866:LYS:HE3	2.09	0.52
1:A:37:ALA:O	1:A:41:MET:HG3	2.09	0.52
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.92	0.52
1:A:220:MET:HA	1:A:223:PHE:CB	2.40	0.52
1:A:586:HIS:CD2	1:A:676:VAL:HG21	2.45	0.52
1:A:191:VAL:HG13	1:A:220:MET:HE3	1.92	0.52
1:A:654:ASP:O	1:A:673:VAL:HG21	2.10	0.52
1:A:833:ILE:HG23	1:A:989:TRP:NE1	2.25	0.52
1:A:1177:LYS:HE3	1:A:1178:ASN:N	2.25	0.52
1:A:548:LYS:HG3	1:A:550:LEU:HD13	1.93	0.51
1:A:837:PRO:HD3	1:A:989:TRP:CD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:LEU:HD12	1:A:600:GLU:O	2.10	0.51
1:A:605:THR:HG23	1:A:606:PRO:HD2	1.91	0.51
1:A:924:MET:HE1	1:A:928:LEU:HD11	1.91	0.51
1:A:220:MET:O	1:A:224:THR:HG23	2.10	0.51
1:A:250:ASN:N	1:A:250:ASN:ND2	2.56	0.51
1:A:800:THR:HG21	1:A:1073:GLY:CA	2.41	0.51
1:A:52:LYS:O	1:A:54:GLY:N	2.43	0.51
1:A:874:THR:HB	1:A:923:ASN:HD21	1.76	0.51
1:A:187:SER:O	1:A:189:GLU:N	2.43	0.51
1:A:372:TYR:CD1	1:A:372:TYR:C	2.88	0.51
1:A:375:ASN:CA	1:A:378:THR:HG22	2.39	0.51
1:A:649:HIS:HB2	1:A:650:PRO:HD2	1.93	0.51
1:A:377:ILE:HD11	1:A:592:GLU:HB3	1.93	0.51
1:A:74:LEU:HD21	1:A:96:VAL:HG13	1.93	0.51
1:A:604:HIS:CE1	1:A:1262:SER:HB3	2.46	0.51
1:A:15:ARG:CZ	1:A:38:ILE:HG21	2.41	0.51
1:A:134:ARG:HG3	1:A:259:PHE:CE1	2.45	0.51
1:A:712:ALA:O	1:A:715:THR:HB	2.11	0.51
1:A:66:ILE:HD13	1:A:66:ILE:H	1.75	0.51
1:A:840:GLU:H	1:A:840:GLU:CD	2.19	0.51
1:A:923:ASN:O	1:A:927:GLN:HG3	2.11	0.51
1:A:35:GLU:O	1:A:38:ILE:HG12	2.11	0.50
1:A:1016:SER:O	1:A:1022:THR:HG21	2.11	0.50
1:A:15:ARG:NH2	1:A:38:ILE:HG21	2.26	0.50
1:A:108:VAL:HG22	1:A:112:LYS:HE3	1.92	0.50
1:A:307:HIS:HD2	1:A:390:VAL:HA	1.75	0.50
1:A:57:ALA:HA	1:A:79:GLN:HB3	1.93	0.50
2:G:2008:C:H2'	5:T:2501:GH3:O4'	2.11	0.50
1:A:297:VAL:HB	1:A:361:TYR:CD1	2.46	0.50
1:A:372:TYR:CD1	1:A:410:VAL:HG21	2.46	0.50
1:A:410:VAL:O	1:A:410:VAL:HG13	2.12	0.50
1:A:598:LYS:HD3	1:A:604:HIS:CB	2.41	0.50
1:A:785:VAL:CG2	1:A:912:THR:HB	2.41	0.50
1:A:862:HIS:CD2	1:A:864:SER:OG	2.64	0.50
1:A:187:SER:O	1:A:190:VAL:HG12	2.11	0.50
1:A:441:LEU:O	1:A:442:LEU:C	2.54	0.50
1:A:930:ILE:HD11	1:A:1021:TYR:HB2	1.94	0.50
1:A:1239:ILE:HG22	1:A:1239:ILE:O	2.11	0.50
1:A:1049:THR:HG22	1:A:1056:ILE:HB	1.93	0.50
1:A:1235:ILE:N	1:A:1235:ILE:HD12	2.26	0.50
1:A:9:VAL:CG1	1:A:23:CYS:HB3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:HIS:O	1:A:373:VAL:HG23	2.12	0.49
1:A:1243:ASN:N	1:A:1243:ASN:HD22	2.10	0.49
1:A:276:VAL:HG11	1:A:352:VAL:HG11	1.93	0.49
1:A:252:GLU:CD	1:A:253:VAL:H	2.21	0.49
1:A:747:ILE:HG12	1:A:747:ILE:O	2.12	0.49
1:A:871:GLN:HB2	1:A:922:TRP:CD1	2.47	0.49
1:A:1118:LEU:CD2	2:G:2005:C:H5''	2.42	0.49
1:A:109:GLU:OE2	1:A:112:LYS:HD2	2.13	0.49
1:A:304:HIS:CE1	1:A:305:VAL:HG12	2.48	0.49
1:A:382:GLN:CD	1:A:382:GLN:C	2.81	0.49
1:A:924:MET:HE1	1:A:928:LEU:CD1	2.42	0.49
1:A:103:GLY:O	1:A:105:ILE:N	2.46	0.49
1:A:354:TYR:CE2	1:A:361:TYR:HB2	2.48	0.49
1:A:134:ARG:HH11	1:A:259:PHE:CB	2.26	0.48
1:A:1023:PHE:O	1:A:1026:GLU:HG2	2.13	0.48
1:A:75:GLU:HB3	1:A:134:ARG:HG2	1.94	0.48
1:A:500:GLU:CD	1:A:1241:ARG:HD3	2.39	0.48
1:A:714:ASN:HD21	1:A:1254:PHE:N	1.89	0.48
1:A:1236:ASP:C	1:A:1238:LEU:N	2.71	0.48
1:A:130:ILE:O	1:A:130:ILE:HG12	2.13	0.48
1:A:188:ALA:O	1:A:192:GLU:HB2	2.12	0.48
1:A:1074:PHE:N	1:A:1074:PHE:CD2	2.78	0.48
1:A:203:MET:HE3	1:A:207:LYS:O	2.14	0.48
1:A:1236:ASP:C	1:A:1238:LEU:H	2.21	0.48
1:A:52:LYS:C	1:A:54:GLY:N	2.72	0.48
1:A:957:GLU:O	1:A:961:THR:HB	2.14	0.48
1:A:984:LEU:HD23	1:A:1029:ILE:HD12	1.94	0.48
1:A:752:ARG:H	1:A:763:ASN:ND2	2.12	0.48
1:A:971:ALA:O	1:A:972:ALA:C	2.57	0.48
1:A:117:GLU:O	1:A:120:VAL:HG22	2.14	0.47
1:A:134:ARG:NH1	1:A:259:PHE:HA	2.28	0.47
1:A:252:GLU:OE2	1:A:253:VAL:N	2.46	0.47
1:A:47:ILE:O	1:A:50:ALA:HB3	2.14	0.47
1:A:80:THR:CG2	1:A:83:VAL:H	2.27	0.47
1:A:1173:ASN:HD22	1:A:1175:PHE:N	2.04	0.47
1:A:1193:ARG:HG2	1:A:1194:ASP:N	2.30	0.47
1:A:376:MET:HG3	1:A:410:VAL:HG22	1.95	0.47
1:A:629:PRO:HD2	1:A:632:VAL:HG13	1.96	0.47
1:A:22:ASP:O	1:A:41:MET:HE3	2.14	0.47
1:A:948:GLN:HE21	1:A:1091:CYS:HB3	1.80	0.47
1:A:200:ASP:O	1:A:201:ILE:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.82	0.47
1:A:198:GLN:HA	1:A:201:ILE:CD1	2.40	0.47
1:A:197:VAL:HG13	1:A:198:GLN:N	2.30	0.47
1:A:65:LYS:CG	1:A:101:VAL:HG21	2.40	0.47
1:A:626:ILE:HG22	1:A:645:VAL:HG22	1.97	0.47
1:A:23:CYS:O	1:A:27:LEU:HB2	2.15	0.46
1:A:413:PRO:HB2	1:A:414:TYR:HD1	1.77	0.46
1:A:596:LEU:CD1	1:A:600:GLU:HB2	2.45	0.46
2:G:2005:C:O2'	2:G:2006:C:H5'	2.14	0.46
1:A:4:ILE:HG22	1:A:5:THR:N	2.29	0.46
1:A:562:LEU:N	1:A:562:LEU:HD12	2.31	0.46
1:A:729:ASN:ND2	1:A:740:PHE:H	2.11	0.46
1:A:34:ILE:HG22	1:A:35:GLU:N	2.30	0.46
1:A:418:PHE:HD1	1:A:476:LEU:HD22	1.80	0.46
1:A:521:ILE:HD12	1:A:525:GLU:OE2	2.15	0.46
1:A:324:TYR:CG	1:A:357:PRO:HD3	2.51	0.46
1:A:324:TYR:CD2	1:A:357:PRO:HG3	2.51	0.46
1:A:493:LYS:HB3	1:A:494:PRO:HD2	1.98	0.46
1:A:812:ASP:O	1:A:813:PHE:C	2.58	0.46
1:A:194:GLU:HA	1:A:197:VAL:HG12	1.98	0.46
1:A:1173:ASN:HD21	1:A:1175:PHE:H	1.58	0.46
1:A:4:ILE:HG22	1:A:5:THR:HG22	1.98	0.46
1:A:472:LYS:O	1:A:475:GLU:HB3	2.16	0.46
1:A:442:LEU:O	1:A:447:PHE:HB2	2.15	0.46
1:A:1262:SER:O	1:A:1264:ARG:N	2.48	0.46
1:A:272:PHE:O	1:A:275:GLU:HB3	2.16	0.46
1:A:363:HIS:C	1:A:363:HIS:CD2	2.93	0.46
1:A:203:MET:HG2	1:A:212:ALA:HB3	1.97	0.46
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.96	0.46
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.83	0.45
1:A:715:THR:HG21	1:A:1149:PRO:HG3	1.97	0.45
1:A:824:MET:CE	1:A:1040:ILE:HD12	2.46	0.45
1:A:833:ILE:HD12	1:A:833:ILE:HA	1.51	0.45
1:A:944:ASP:OD2	1:A:944:ASP:C	2.57	0.45
3:T:2109:C:H2'	3:T:2110:C:C6	2.51	0.45
1:A:15:ARG:HH12	1:A:38:ILE:HD13	1.81	0.45
1:A:717:ILE:HD13	1:A:717:ILE:O	2.15	0.45
1:A:832:LEU:HG	1:A:833:ILE:HD13	1.98	0.45
1:A:874:THR:HG22	1:A:877:ALA:CB	2.46	0.45
1:A:60:GLY:HA3	1:A:77:ASN:HB2	1.99	0.45
1:A:418:PHE:CD1	1:A:476:LEU:HD22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:ASN:C	1:A:901:ASN:ND2	2.73	0.45
1:A:260:GLU:HB3	1:A:263:GLU:HG3	1.99	0.45
1:A:372:TYR:CE1	1:A:376:MET:HB2	2.51	0.45
1:A:445:TYR:O	1:A:446:ASP:HB2	2.16	0.45
1:A:1206:ASP:OD1	1:A:1210:ARG:HD2	2.17	0.45
1:A:49:ALA:HA	1:A:52:LYS:HB2	1.99	0.45
1:A:172:HIS:C	1:A:172:HIS:CD2	2.95	0.45
1:A:301:THR:HG23	1:A:365:ASP:OD2	2.17	0.45
1:A:49:ALA:HB2	1:A:123:VAL:CG1	2.40	0.45
1:A:253:VAL:HG23	1:A:253:VAL:O	2.17	0.45
1:A:571:ILE:HG22	1:A:572:GLU:N	2.32	0.45
1:A:1077:ASN:C	1:A:1077:ASN:ND2	2.75	0.45
1:A:1145:ARG:HH11	1:A:1145:ARG:HB3	1.82	0.45
3:T:2109:C:H2'	3:T:2110:C:H6	1.81	0.45
1:A:502:VAL:HG21	1:A:571:ILE:HB	1.99	0.45
1:A:80:THR:HG22	1:A:83:VAL:HG23	1.99	0.44
1:A:118:GLU:O	1:A:121:ALA:HB3	2.17	0.44
1:A:782:THR:HG23	1:A:784:ALA:HB3	1.99	0.44
1:A:66:ILE:HG12	1:A:66:ILE:O	2.16	0.44
1:A:320:LEU:HD12	1:A:355:ASP:O	2.17	0.44
1:A:728:ALA:O	1:A:732:LEU:HG	2.18	0.44
1:A:614:GLN:HG3	1:A:621:ASP:HB3	1.99	0.44
1:A:733:LEU:HD12	1:A:733:LEU:HA	1.86	0.44
1:A:1124:TYR:CE1	1:A:1128:THR:HG21	2.52	0.44
1:A:107:ASP:HB3	1:A:110:VAL:HG23	2.00	0.44
1:A:772:LYS:HE3	1:A:1105:TYR:CE1	2.52	0.44
1:A:53:ALA:HA	1:A:129:ASN:CG	2.43	0.44
1:A:181:ILE:HD12	1:A:253:VAL:O	2.18	0.44
1:A:765:LEU:HD12	1:A:765:LEU:HA	1.81	0.44
1:A:998:SER:HA	1:A:999:PRO:HD2	1.86	0.44
1:A:121:ALA:O	1:A:125:LYS:HG3	2.17	0.44
1:A:220:MET:H	1:A:220:MET:HG2	1.59	0.44
1:A:229:LEU:HD11	1:A:242:VAL:HG11	2.00	0.44
1:A:629:PRO:HD2	1:A:632:VAL:HG11	1.99	0.44
1:A:956:HIS:O	1:A:960:VAL:HG12	2.18	0.44
1:A:12:LEU:HG	1:A:23:CYS:SG	2.57	0.44
1:A:836:VAL:CG2	1:A:837:PRO:HD2	2.48	0.44
1:A:65:LYS:HG2	1:A:101:VAL:CG2	2.42	0.44
1:A:147:GLN:HG3	1:A:149:GLY:O	2.18	0.44
1:A:210:GLU:HA	1:A:213:GLU:HB2	2.00	0.44
1:A:20:MET:HA	1:A:20:MET:CE	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:O	1:A:166:VAL:HG22	2.18	0.43
1:A:384:ASP:O	1:A:413:PRO:HD2	2.17	0.43
1:A:1057:LEU:N	1:A:1057:LEU:HD23	2.32	0.43
1:A:222:LYS:O	1:A:223:PHE:C	2.60	0.43
1:A:1003:LEU:HB3	1:A:1004:PRO:CD	2.48	0.43
1:A:500:GLU:CD	1:A:1210:ARG:NH1	2.75	0.43
1:A:276:VAL:CG1	1:A:277:ALA:N	2.81	0.43
1:A:700:SER:O	1:A:1179:ARG:CD	2.63	0.43
1:A:773:TYR:CE2	1:A:775:ASP:HB3	2.54	0.43
1:A:868:ALA:HB2	1:A:1201:GLY:HA3	1.99	0.43
1:A:21:MET:O	1:A:25:LYS:HG2	2.19	0.43
1:A:496:LEU:HA	1:A:577:LEU:O	2.19	0.43
1:A:936:ASP:O	1:A:939:ARG:HB2	2.18	0.43
1:A:806:ARG:N	1:A:807:PRO:CD	2.82	0.43
1:A:1021:TYR:CD1	1:A:1021:TYR:C	2.95	0.43
2:G:2001:G:H2'	2:G:2002:G:H8	1.83	0.43
1:A:152:ILE:HD13	1:A:258:ARG:NH1	2.33	0.43
1:A:134:ARG:HH11	1:A:259:PHE:CA	2.31	0.43
1:A:1003:LEU:HB3	1:A:1004:PRO:HD2	2.00	0.43
1:A:1262:SER:O	1:A:1263:SER:C	2.61	0.43
1:A:1019:ASN:CB	1:A:1022:THR:HG22	2.19	0.43
1:A:210:GLU:CD	1:A:210:GLU:N	2.72	0.42
1:A:1035:ARG:NH2	6:A:3515:HOH:O	2.52	0.42
1:A:1093:LYS:HA	1:A:1093:LYS:HD3	1.78	0.42
1:A:1185:VAL:HG11	1:A:1261:CYS:SG	2.59	0.42
1:A:4:ILE:HG22	1:A:5:THR:CG2	2.50	0.42
1:A:1154:ARG:HH11	1:A:1154:ARG:CG	2.12	0.42
1:A:1172:ILE:HD13	1:A:1172:ILE:HA	1.88	0.42
1:A:165:LEU:HA	1:A:165:LEU:HD22	1.76	0.42
1:A:791:LEU:HD12	1:A:791:LEU:HA	1.69	0.42
1:A:1128:THR:O	1:A:1128:THR:CG2	2.65	0.42
1:A:61:VAL:HG13	1:A:89:PHE:HE1	1.83	0.42
1:A:194:GLU:O	1:A:197:VAL:HG12	2.19	0.42
1:A:305:VAL:HG13	1:A:306:ASP:H	1.85	0.42
1:A:906:VAL:O	1:A:913:ASP:HB3	2.19	0.42
1:A:1173:ASN:ND2	1:A:1173:ASN:C	2.67	0.42
1:A:93:ALA:HA	1:A:96:VAL:CG1	2.48	0.42
1:A:200:ASP:O	1:A:203:MET:N	2.53	0.42
1:A:246:LEU:HD21	1:A:253:VAL:HG13	2.00	0.42
1:A:628:LEU:HD12	1:A:628:LEU:HA	1.81	0.42
1:A:817:LEU:HD23	1:A:1067:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:MET:HE1	1:A:1040:ILE:HG13	2.00	0.42
1:A:837:PRO:HD3	1:A:989:TRP:CE2	2.55	0.42
1:A:1177:LYS:HE3	1:A:1177:LYS:CA	2.49	0.42
1:A:435:GLU:O	1:A:439:ARG:HG3	2.20	0.42
1:A:567:LYS:HD2	1:A:569:GLU:OE2	2.18	0.42
1:A:812:ASP:O	1:A:814:ASN:N	2.53	0.42
1:A:649:HIS:CB	1:A:650:PRO:CD	2.97	0.42
1:A:777:SER:O	1:A:779:GLY:N	2.52	0.42
1:A:586:HIS:CG	1:A:676:VAL:HG21	2.55	0.42
1:A:924:MET:HE3	1:A:924:MET:C	2.45	0.42
1:A:222:LYS:O	1:A:225:GLY:N	2.53	0.42
1:A:356:THR:O	1:A:357:PRO:C	2.60	0.41
1:A:420:ASN:CG	1:A:421:LYS:N	2.78	0.41
1:A:579:LYS:HA	1:A:580:PRO:HD3	1.87	0.41
1:A:860:TYR:HA	1:A:865:PHE:CD1	2.55	0.41
1:A:1054:ASP:OD1	1:A:1091:CYS:N	2.44	0.41
1:A:465:GLY:HA2	1:A:470:GLU:OE2	2.19	0.41
1:A:38:ILE:HG13	1:A:39:GLU:N	2.34	0.41
1:A:235:VAL:CG1	1:A:608:PHE:HZ	2.33	0.41
1:A:304:HIS:ND1	1:A:305:VAL:HG12	2.36	0.41
1:A:1092:GLY:HA3	2:G:2007:A:H4'	2.01	0.41
1:A:74:LEU:HD12	1:A:75:GLU:H	1.85	0.41
1:A:304:HIS:HD2	1:A:397:MET:HE2	1.84	0.41
1:A:712:ALA:HB1	1:A:1152:LEU:HD22	2.02	0.41
1:A:996:LEU:HD12	1:A:996:LEU:HA	1.77	0.41
1:A:419:LEU:HD23	1:A:454:ILE:HG23	2.02	0.41
1:A:1116:LEU:HD13	1:A:1148:LEU:HG	2.03	0.41
1:A:436:MET:HE3	1:A:436:MET:HB2	1.93	0.41
1:A:521:ILE:O	1:A:552:GLU:HA	2.21	0.41
1:A:724:ALA:HB1	1:A:1106:ILE:HG21	2.03	0.41
1:A:846:CYS:HB3	1:A:925:PHE:CE2	2.56	0.41
1:A:994:MET:HE3	1:A:994:MET:HB3	1.88	0.41
1:A:785:VAL:HG22	1:A:912:THR:HB	2.02	0.41
1:A:10:LYS:HD3	1:A:433:LEU:HD11	2.03	0.41
1:A:64:THR:HB	1:A:147:GLN:NE2	2.36	0.41
1:A:165:LEU:O	1:A:169:ILE:HG23	2.21	0.41
1:A:275:GLU:OE2	1:A:275:GLU:O	2.39	0.41
1:A:304:HIS:HB3	1:A:307:HIS:CG	2.56	0.41
1:A:658:ARG:NH1	1:A:672:VAL:HG11	2.35	0.41
1:A:195:TYR:O	1:A:199:LEU:HB2	2.21	0.41
1:A:273:ALA:HA	1:A:352:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:HA	1:A:295:PRO:HD3	1.91	0.40
1:A:300:GLY:CA	1:A:383:MET:SD	3.07	0.40
1:A:596:LEU:HD13	1:A:600:GLU:HB2	2.02	0.40
1:A:636:MET:O	1:A:637:PRO:C	2.63	0.40
1:A:797:CYS:HB2	1:A:1012:GLU:HB3	2.02	0.40
1:A:1057:LEU:HD23	1:A:1057:LEU:H	1.84	0.40
1:A:97:LEU:O	1:A:100:ALA:N	2.51	0.40
1:A:199:LEU:O	1:A:203:MET:HB2	2.22	0.40
1:A:273:ALA:O	1:A:274:ALA:C	2.62	0.40
1:A:460:LEU:O	1:A:464:GLU:HG3	2.21	0.40
1:A:521:ILE:O	1:A:521:ILE:HG23	2.22	0.40
1:A:878:LEU:HD22	1:A:897:ILE:HD12	2.03	0.40
1:A:950:ILE:O	1:A:950:ILE:HD12	2.21	0.40
1:A:134:ARG:HH11	1:A:259:PHE:HA	1.85	0.40
1:A:703:ASN:C	1:A:705:LEU:N	2.79	0.40
1:A:1003:LEU:HD12	1:A:1003:LEU:N	2.37	0.40
1:A:180:PHE:CD2	1:A:186:VAL:HG12	2.56	0.40
1:A:234:PHE:CE1	1:A:236:MET:HB2	2.56	0.40
1:A:874:THR:HG21	6:A:3505:HOH:O	2.20	0.40
1:A:1122:ASN:HD22	1:A:1122:ASN:HA	1.70	0.40
1:A:34:ILE:HD12	1:A:34:ILE:N	2.35	0.40
1:A:529:ILE:HD13	1:A:529:ILE:C	2.46	0.40
1:A:1237:GLN:C	1:A:1239:ILE:H	2.29	0.40
2:G:2004:U:H2'	2:G:2005:C:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1193/1289 (93%)	1070 (90%)	100 (8%)	23 (2%)	6 13

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	104	LYS
1	A	250	ASN
1	A	381	ALA
1	A	806	ARG
1	A	810	SER
1	A	813	PHE
1	A	1263	SER
1	A	188	ALA
1	A	223	PHE
1	A	778	LEU
1	A	53	ALA
1	A	187	SER
1	A	273	ALA
1	A	324	TYR
1	A	325	GLY
1	A	535	THR
1	A	201	ILE
1	A	467	ALA
1	A	703	ASN
1	A	619	THR
1	A	209	LYS
1	A	780	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	995/1060 (94%)	832 (84%)	163 (16%)	2 4

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	9	VAL

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Mol	Chain	Res	Type
1	A	24	LYS
1	A	40	ASN
1	A	56	VAL
1	A	61	VAL
1	A	64	THR
1	A	66	ILE
1	A	76	VAL
1	A	80	THR
1	A	81	ASP
1	A	111	LEU
1	A	122	LEU
1	A	130	ILE
1	A	133	ARG
1	A	151	ARG
1	A	154	VAL
1	A	155	LEU
1	A	156	VAL
1	A	165	LEU
1	A	166	VAL
1	A	169	ILE
1	A	181	ILE
1	A	189	GLU
1	A	196	GLN
1	A	203	MET
1	A	205	SER
1	A	210	GLU
1	A	230	THR
1	A	235	VAL
1	A	237	GLU
1	A	245	LEU
1	A	246	LEU
1	A	250	ASN
1	A	254	THR
1	A	258	ARG
1	A	269	GLU
1	A	282	GLN
1	A	292	ARG
1	A	305	VAL
1	A	307	HIS
1	A	310	THR
1	A	320	LEU
1	A	352	VAL

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Mol	Chain	Res	Type
1	A	356	THR
1	A	364	VAL
1	A	371	ASP
1	A	387	ILE
1	A	390	VAL
1	A	399	GLN
1	A	401	ARG
1	A	406	LEU
1	A	410	VAL
1	A	419	LEU
1	A	438	VAL
1	A	440	GLU
1	A	452	THR
1	A	455	VAL
1	A	480	LEU
1	A	491	ILE
1	A	497	LEU
1	A	502	VAL
1	A	508	ARG
1	A	511	VAL
1	A	516	VAL
1	A	522	LYS
1	A	529	ILE
1	A	530	VAL
1	A	535	THR
1	A	547	ARG
1	A	549	LEU
1	A	550	LEU
1	A	563	LEU
1	A	568	ARG
1	A	571	ILE
1	A	582	THR
1	A	593	VAL
1	A	604	HIS
1	A	614	GLN
1	A	619	THR
1	A	622	VAL
1	A	626	ILE
1	A	628	LEU
1	A	632	VAL
1	A	646	THR
1	A	672	VAL

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Mol	Chain	Res	Type
1	A	676	VAL
1	A	715	THR
1	A	717	ILE
1	A	731	LEU
1	A	733	LEU
1	A	747	ILE
1	A	777	SER
1	A	778	LEU
1	A	782	THR
1	A	785	VAL
1	A	791	LEU
1	A	799	LEU
1	A	800	THR
1	A	804	LEU
1	A	809	TYR
1	A	833	ILE
1	A	835	ASP
1	A	839	VAL
1	A	842	MET
1	A	843	LEU
1	A	847	ARG
1	A	854	THR
1	A	858	ARG
1	A	869	LEU
1	A	873	CYS
1	A	874	THR
1	A	894	ILE
1	A	901	ASN
1	A	906	VAL
1	A	916	ILE
1	A	930	ILE
1	A	933	ILE
1	A	938	LEU
1	A	943	ILE
1	A	949	THR
1	A	950	ILE
1	A	960	VAL
1	A	961	THR
1	A	967	VAL
1	A	970	SER
1	A	973	SER
1	A	984	LEU

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Mol	Chain	Res	Type
1	A	996	LEU
1	A	1012	GLU
1	A	1013	LYS
1	A	1014	ILE
1	A	1022	THR
1	A	1033	LEU
1	A	1040	ILE
1	A	1049	THR
1	A	1053	ASP
1	A	1075	THR
1	A	1076	THR
1	A	1089	GLU
1	A	1099	VAL
1	A	1102	THR
1	A	1116	LEU
1	A	1128	THR
1	A	1145	ARG
1	A	1151	GLN
1	A	1152	LEU
1	A	1154	ARG
1	A	1173	ASN
1	A	1177	LYS
1	A	1182	ILE
1	A	1189	THR
1	A	1194	ASP
1	A	1200	LEU
1	A	1204	LEU
1	A	1236	ASP
1	A	1237	GLN
1	A	1241	ARG
1	A	1243	ASN
1	A	1250	SER
1	A	1251	THR
1	A	1257	GLN
1	A	1261	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	114	GLN
1	A	147	GLN

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Mol	Chain	Res	Type
1	A	250	ASN
1	A	282	GLN
1	A	298	ASN
1	A	307	HIS
1	A	382	GLN
1	A	399	GLN
1	A	403	HIS
1	A	409	GLN
1	A	536	GLN
1	A	586	HIS
1	A	640	ASN
1	A	708	GLN
1	A	714	ASN
1	A	729	ASN
1	A	763	ASN
1	A	862	HIS
1	A	871	GLN
1	A	901	ASN
1	A	946	ASN
1	A	948	GLN
1	A	1077	ASN
1	A	1121	ASN
1	A	1122	ASN
1	A	1138	HIS
1	A	1151	GLN
1	A	1155	ASN
1	A	1173	ASN
1	A	1237	GLN
1	A	1243	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	6/8 (75%)	1 (16%)	0
3	T	11/12 (91%)	2 (18%)	0
All	All	17/20 (85%)	3 (17%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	2002	G

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Mol	Chain	Res	Type
3	T	2102	U
3	T	2111	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GH3	T	2501	4	31,33,33	2.54	12 (38%)	44,52,52	2.38	16 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GH3	T	2501	4	-	5/22/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	2501	GH3	O6-C6	7.87	1.38	1.23
5	T	2501	GH3	C2-N2	6.55	1.49	1.34
5	T	2501	GH3	C5-N7	-3.65	1.31	1.39
5	T	2501	GH3	C8-N9	-3.37	1.30	1.37
5	T	2501	GH3	PB-O3B	-3.22	1.56	1.59
5	T	2501	GH3	C8-N7	-2.94	1.24	1.32
5	T	2501	GH3	C5-C4	2.79	1.46	1.38
5	T	2501	GH3	C4-N9	2.49	1.44	1.38
5	T	2501	GH3	C3'-C4'	-2.19	1.48	1.52
5	T	2501	GH3	C5-C6	-2.12	1.36	1.44
5	T	2501	GH3	C3'-C2'	-2.04	1.47	1.52
5	T	2501	GH3	O2'-C2'	-2.04	1.39	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	2501	GH3	N9-C4-N3	6.62	139.19	125.95
5	T	2501	GH3	C1'-N9-C4	-4.88	112.06	126.49
5	T	2501	GH3	C5-C4-N3	-4.50	121.23	128.39
5	T	2501	GH3	C8-N7-C5	4.32	111.96	104.26
5	T	2501	GH3	C1'-N9-C8	4.26	138.84	126.73
5	T	2501	GH3	O2B-PB-O3A	4.25	118.76	107.27
5	T	2501	GH3	O6-C6-C5	-3.96	116.09	126.53
5	T	2501	GH3	C2-N3-C4	3.56	118.44	112.30
5	T	2501	GH3	C5-C4-N9	-3.41	99.54	105.66
5	T	2501	GH3	O2G-PG-O3B	3.24	115.50	104.64
5	T	2501	GH3	O4'-C1'-N9	3.04	115.24	108.36
5	T	2501	GH3	C5-C6-N1	2.58	119.83	113.25
5	T	2501	GH3	C2-N1-C6	-2.56	120.47	125.11
5	T	2501	GH3	C6-C5-N7	2.42	134.69	130.29
5	T	2501	GH3	O6-C6-N1	2.11	124.08	120.11
5	T	2501	GH3	O4'-C1'-C2'	-2.11	104.53	106.51

There are no chirality outliers.

All (5) torsion outliers are listed below:

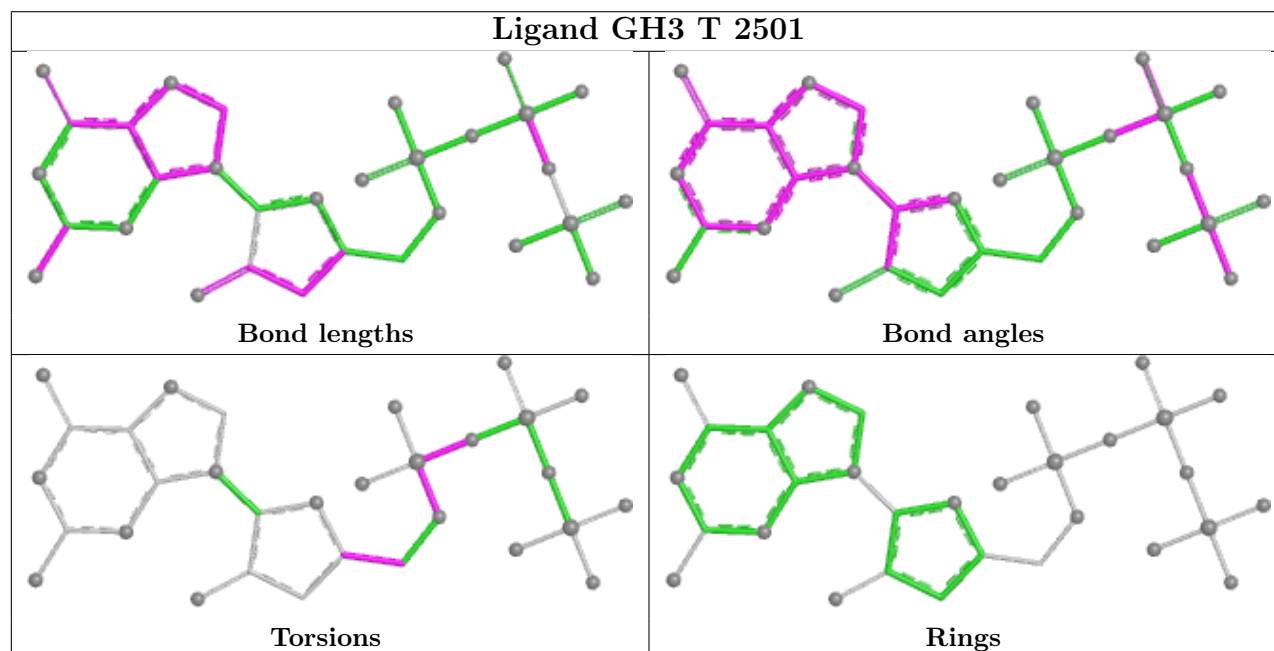
Mol	Chain	Res	Type	Atoms
5	T	2501	GH3	PB-O3A-PA-O5'
5	T	2501	GH3	C5'-O5'-PA-O3A
5	T	2501	GH3	C5'-O5'-PA-O2A
5	T	2501	GH3	O4'-C4'-C5'-O5'
5	T	2501	GH3	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	2501	GH3	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1203/1289 (93%)	-0.40	16 (1%) 75 71	20, 51, 100, 127	0
2	G	8/8 (100%)	-0.52	0 100 100	35, 52, 83, 84	0
3	T	12/12 (100%)	-0.56	0 100 100	30, 49, 90, 118	0
All	All	1223/1309 (93%)	-0.40	16 (1%) 75 71	20, 51, 100, 127	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	778	LEU	4.8
1	A	1234	ALA	4.3
1	A	199	LEU	3.8
1	A	348	ASN	3.6
1	A	780	ILE	3.1
1	A	190	VAL	2.9
1	A	290	PHE	2.6
1	A	807	PRO	2.5
1	A	202	ALA	2.5
1	A	2	ALA	2.5
1	A	703	ASN	2.4
1	A	701	SER	2.3
1	A	896	ASP	2.3
1	A	205	SER	2.1
1	A	680	ALA	2.1
1	A	191	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

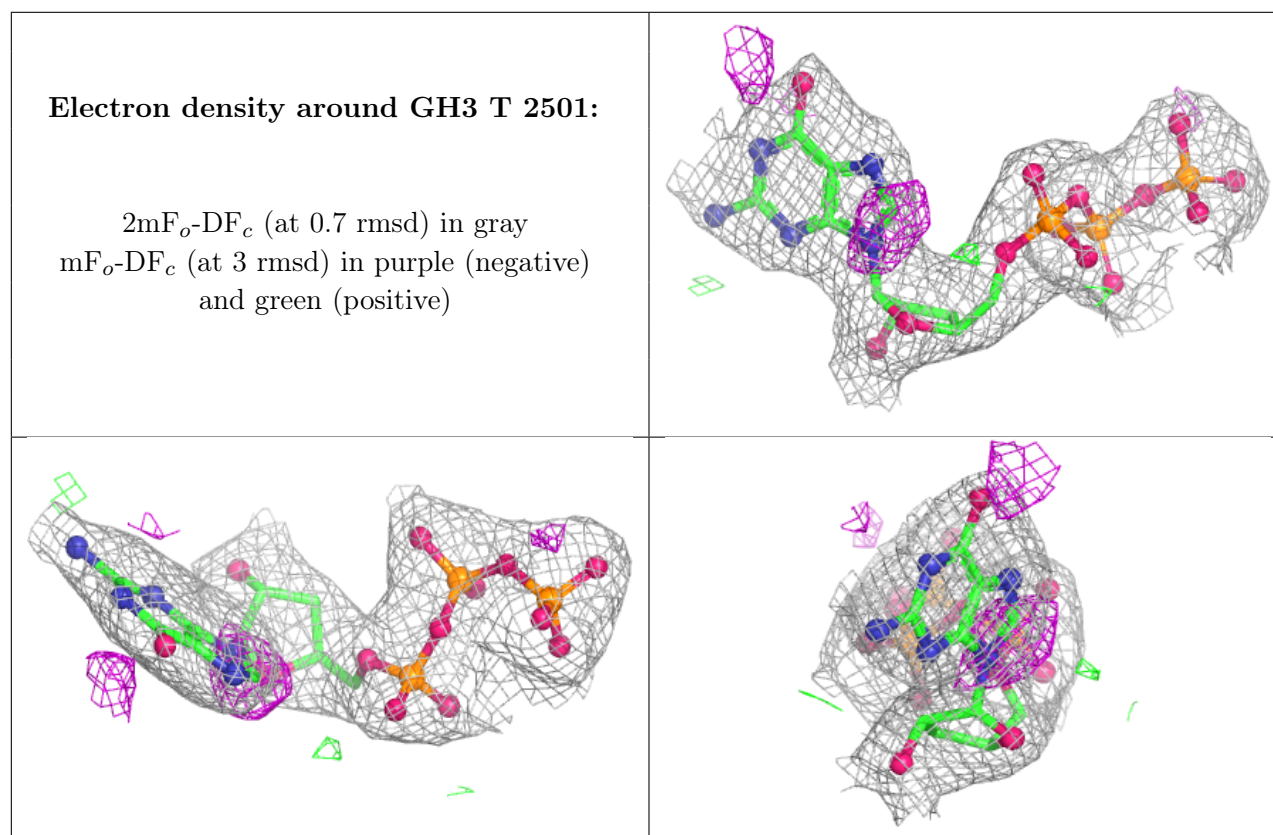
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	A	3002	1/1	0.91	0.12	61,61,61,61	0
5	GH3	T	2501	31/31	0.97	0.06	29,33,39,39	0
4	CA	A	3001	1/1	0.98	0.03	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.